Tatarinoid B

Inchi:	InChI=1S/C12H16O5/c1-7(13)12(14)8-5-10(16-3)11(17-4)6-9(8)15-2/h5-6,12,14H,1-4H3
InchiKey:	LVZSTCWLAWIFNV-UHFFFAOYSA-N
Formula:	C12H16O5
SMILES:	COc1cc(OC)c(C(O)C(C)=O)cc1OC
Mol. weight [g/mol]:	240.25
CAS:	1229005-36-0

Physical Properties

Property code	Value	Unit	Source
gf	-449.50	kJ/mol	Joback Method
hf	-755.64	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	76.83	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.335		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1847.20		NIST Webbook
tb	728.45	K	Joback Method
tc	925.99	K	Joback Method
tf	451.42	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.35	J/mol×K	728.45	Joback Method
cpg	550.77	J/mol×K	893.07	Joback Method
cpg	541.77	J/mol×K	860.15	Joback Method
cpg	532.02	J/mol×K	827.22	Joback Method
cpg	521.51	J/mol×K	794.30	Joback Method
cpg	510.28	J/mol×K	761.37	Joback Method
cpg	558.98	J/mol×K	925.99	Joback Method
dvisc	0.0000233	Pa×s	728.45	Joback Method

dvisc	0.0000329	Pa×s	682.28	Joback Method
dvisc	0.0000487	Pa×s	636.11	Joback Method
dvisc	0.0000767	Pa×s	589.93	Joback Method
dvisc	0.0001305	Pa×s	543.76	Joback Method
dvisc	0.0002449	Pa×s	497.59	Joback Method
dvisc	0.0005228	Pa×s	451.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1229005360&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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